

Introduction to Differentiable Probabilistic Models

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Primer: Standard Machine Learning

- Usually, we are given a set $\mathcal{D} = \{X, y\}$

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ x_{21} & x_{22} & \dots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

where X is our data matrix, and y are our labels.

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where X is our data matrix, and y are our labels.

- Attempt to fit a model f parameterized by θ with respect to an objective function \mathcal{L}

$$\theta^* = \operatorname{argmin}_{\theta} \mathcal{L}(f(X; \theta), y)$$

Reframed as a Probabilistic Model

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- ▶ Examples:
 - ▶ Classification: Fitting two multinomial distributions
 - ▶ Regression: Fitting a Normal centered around the line of best fit

How do we "fit" Distributions?

- ▶ Fitting two distributions implies minimizing their difference, i.e. "distance"
- ▶ This "distance" is known as the divergence between the true distribution P and the learned distribution Q .

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- ▶ Fitting two distributions implies minimizing their difference, i.e. "distance"
- ▶ This "distance" is known as the divergence between the true distribution P and the learned distribution Q .
- ▶ Divergences must satisfy 2 properties:
 - ▶ $D(P \parallel Q) \geq 0 \quad \forall P, Q \in S$
 - ▶ $D(P \parallel Q) = 0 \iff P = Q$

The Kullback-Leibler Divergence

- ▶ The KL Divergence for distributions P and Q is defined as:

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx$$

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- ▶ Note: the KL Divergence is NOT symmetric:

$$D_{KL}(P \parallel Q) \neq D_{KL}(Q \parallel P)$$

- ▶ But we will come back to this later...

Directionality: Forward KL

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- ▶ Note: Maximum Likelihood Estimation is equivalent to minimizing the Forward KL

Digression: Implementing Expectations

$$\begin{aligned} D_{KL}(P \parallel Q) &= \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx \\ &= \mathbb{E}_{x \sim P} \left[\log \left(\frac{p(x)}{q(x)} \right) \right] \end{aligned}$$

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Algorithm 2 $\mathbb{E}_{x \sim P}[f(x)]$

Expectation of $f(x)$ with respect to P

- 1: $x_1, \dots, x_n \sim P$ independently
 - 2: **return** $\frac{1}{N} \sum_{x_i} f(x_i)$
-

Digression: KL to Cross-Entropy

- The KL Divergence can be decomposed into familiar terms:

$$\operatorname{argmin}_Q D_{KL}(P \parallel Q) = \operatorname{argmin}_Q \sum_{x \in \mathcal{X}} p(x) \log \left(\frac{p(x)}{q(x)} \right)$$

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Digression: KL to Cross-Entropy

- ▶ If we consider $P(y_i = 1|x_i) = p_i$ and $Q(y_i = 1|x_i) = \sigma(f_\theta(x_i))$:

$$\operatorname{argmin}_{\theta} D_{KL}(P \parallel Q) =$$

$$\operatorname{argmin}_{\theta} - \left[p_i \log \sigma(f_\theta(x_i)) + (1 - p_i) \log(1 - \sigma(f_\theta(x_i))) \right]$$

- ▶ This is the Binary Cross-Entropy Loss

Forward KL: Learning a Normal Distribution (Initial)

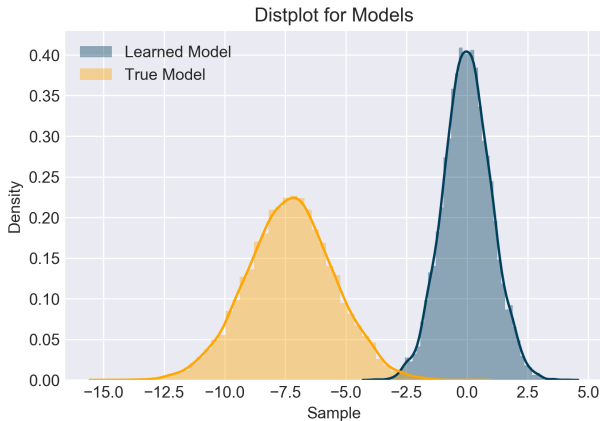


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(0, 1)$

Forward KL: Learning a Normal Distribution (Results)

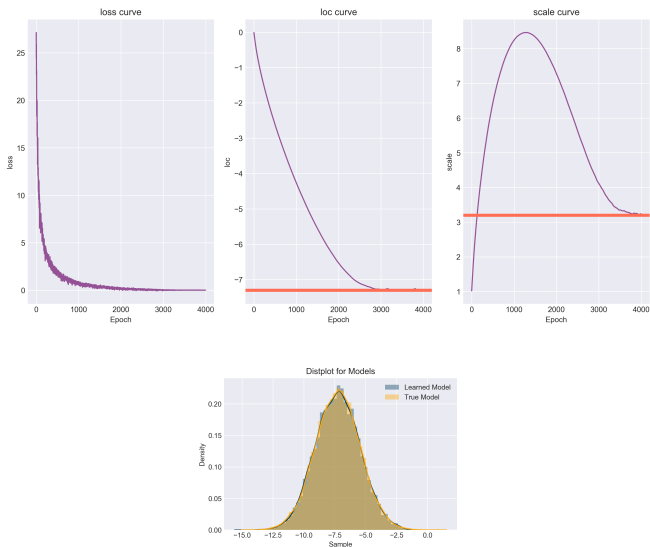


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(-7.28, 3.24)$

Digression: Gaussian Mixture Models

- ▶ We can build a K multi-modal distribution, with weights π , as follows:

$$\begin{aligned}z &\sim \text{Categorical}(\pi) \\ x | z = k &\sim \text{Normal}(\mu_k, \sigma_k)\end{aligned}$$

- ▶ We can calculate log probabilities by marginalizing out z :

$$\log p(x) = \log \sum_{k=1}^K \underbrace{p(z = k)}_{\text{Categorical}} \cdot \underbrace{p(x | z = k)}_{\text{Normal}}$$

Digression: Mixture Models (Visual)

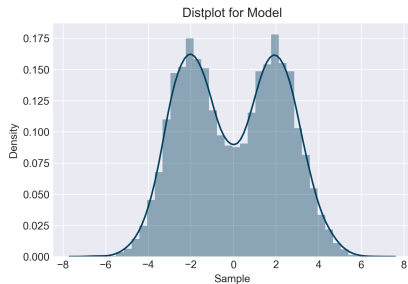


Figure: 2 Mixture Components,
Even Weights

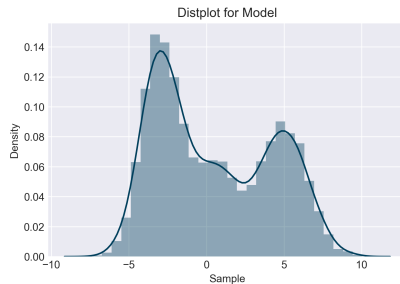


Figure: 3 Mixture Components,
Uneven Weights

Forward KL: Learning a Bimodal (Initial)

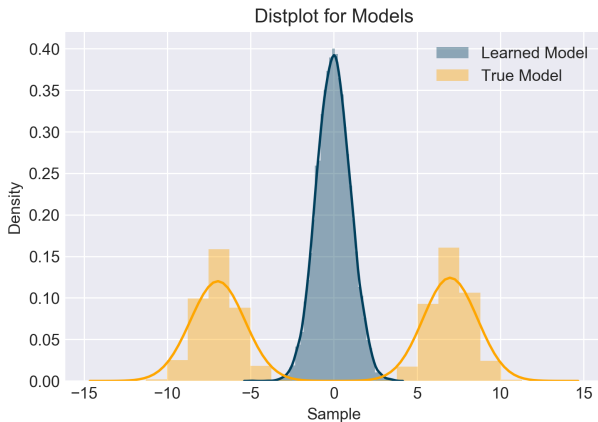


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(0, 1)$

Forward KL: Learning a Bimodal (Results)

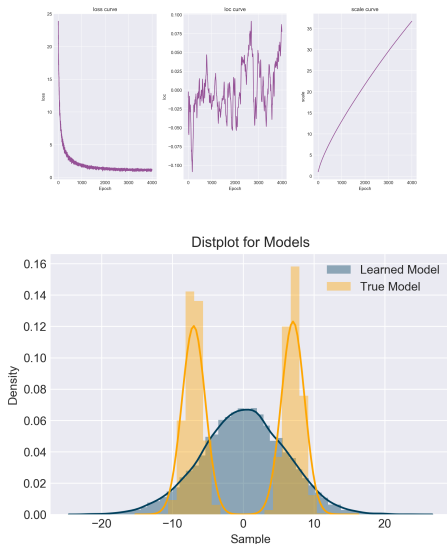


Figure: $Q \sim \mathcal{N}(0.08, 36.76)$

Forward KL: Zero-Avoiding

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} \overbrace{p(x)}^{\text{Constant}} \log \left(\frac{\overbrace{p(x)}^{\text{Constant}}}{\underbrace{q(x)}_{\text{Variable}}} \right) dx$$

- ▶ $p(x)$ is constant-valued, $q(x)$ is variable
- ▶ If Q does not support P , then we will sample a point that has a low probability with respect to Q

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- ▶ $p(x)$ is constant-valued, $q(x)$ is variable
- ▶ If Q does not support P , then we will sample a point that has a low probability with respect to Q
- ▶ As $q(x) \rightarrow 0$, our loss $D_{KL} \rightarrow \infty$
- ▶ Hence, the optimal solution is for Q to cover P , i.e. averaging

Forward KL: Loss Landscape

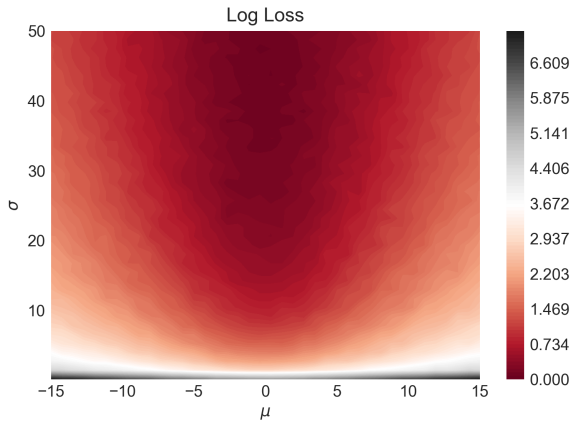


Figure: Loss Landscape for Forward KL Divergence

Directionality: Reverse KL

$$\begin{aligned} D_{KL}(Q \parallel P) &= \int_{-\infty}^{\infty} q(x) \log \left(\frac{q(x)}{p(x)} \right) dx \\ &= \mathbb{E}_{x \sim Q} \left[\log \left(\frac{q(x)}{p(x)} \right) \right] \end{aligned}$$

- ▶ The Reverse KL will sample from Q , and evaluate the log probabilities from P and Q
- ▶ Recall: KL Divergence is not symmetric, and this has drastic implications...

Digression: Differentiable Sampling via the Reparameterization Trick

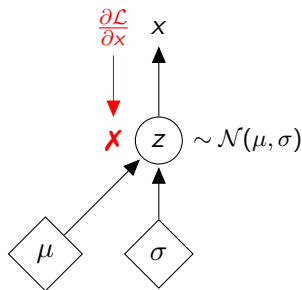


Figure: Original Form

Digression: Differentiable Sampling via the Reparameterization Trick

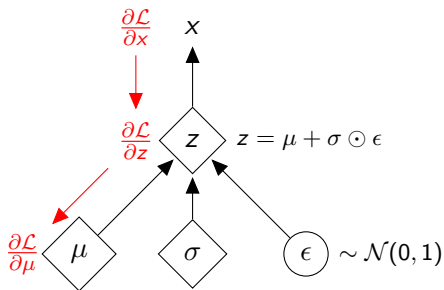


Figure: Reparameterized Version

Digression: Common Reparameterization Tricks

	Reparameterized
$\text{Normal}(\mu, \sigma)$	$\mu + \sigma \cdot \text{Normal}(0, 1)$
$\text{Uniform}(a, b)$	$a + (b - a) \cdot \text{Uniform}(0, 1)$
$\text{Exp}(\lambda)$	$\text{Exp}(1)/\lambda$
$\text{Cauchy}(\mu, \gamma)$	$\mu + \gamma \cdot \text{Cauchy}(0, 1)$

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$\text{Laplace}(\mu, b)$	$u \sim \text{Uniform}(-1, 1)$ $\mu - b \cdot \text{sgn}(u) \cdot \ln[- u + 1]$

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$\text{Categorical}(\pi)$	X

Reverse KL: Learning a Bimodal (Initial)

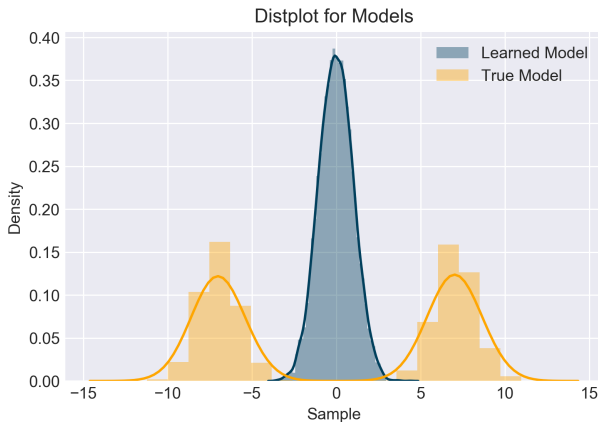


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
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Reverse KL: Learning a Bimodal (Results)

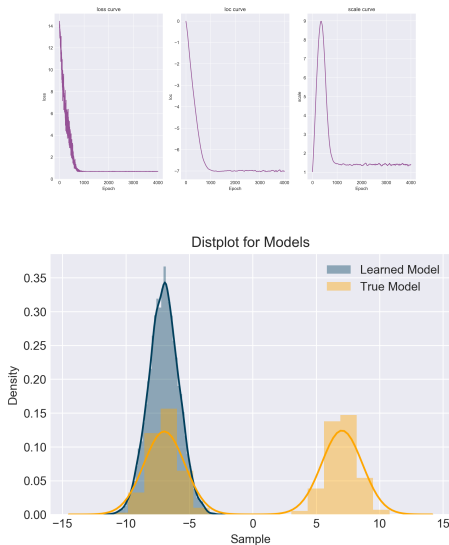


Figure: $Q \sim \mathcal{N}(-7.02, 1.41)$

Reverse KL: Learning a Bimodal Attempt 2 (Results)

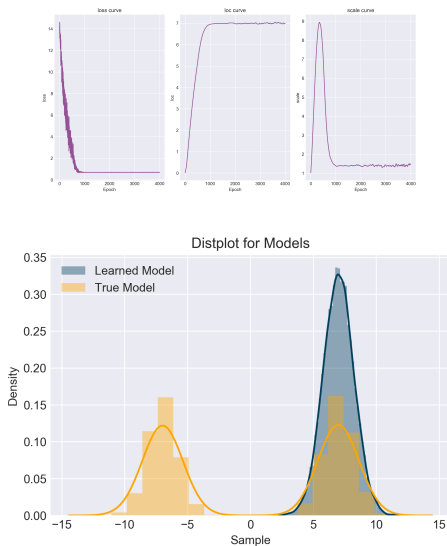


Figure: $Q \sim \mathcal{N}(7.01, 1.46)$

Reverse KL: Zero-Forcing

$$D_{KL}(Q \parallel P) = \int_{-\infty}^{\infty} q(x) \log \left(\frac{q(x)}{p(x)} \right) dx$$

- ▶ Unlike the Forward KL, Reverse KL is Zero-forcing
- ▶ Why? Because we no longer suffer a penalty from $q(x) = 0$
- ▶ However, if $p(x) = 0$, then the optimal value for $q(x)$ is 0
- ▶ Result \implies Mode Collapse

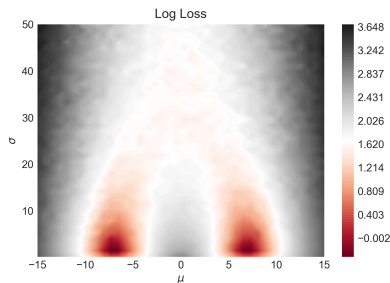


Figure: Loss Landscape for Reverse KL Divergence

Jensen - Shannon Divergence: A Symmetric Divergence

$$\begin{aligned} \text{JSD}(P \parallel Q) &= \frac{1}{2}D_{KL}(P \parallel M) + \frac{1}{2}D_{KL}(Q \parallel M) \\ M &= \frac{1}{2}(P + Q) \end{aligned}$$

- ▶ The JS Divergence is a symmetrized version of the KL Divergence
- ▶ M is the average of distributions P and Q , and can be represented as a Mixture Model

Jensen - Shannon Divergence: Bimodal (Initial)

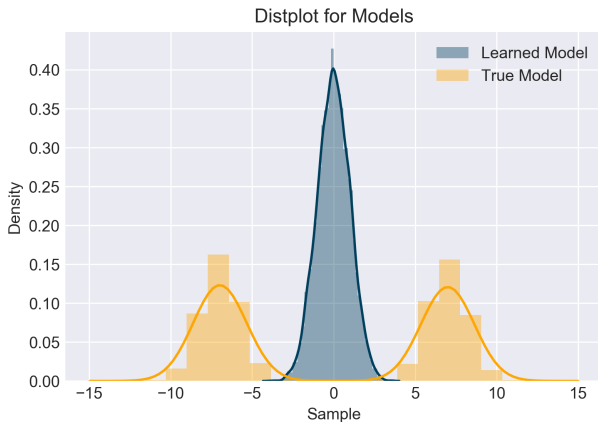


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(0, 1)$

Jensen - Shannon Divergence: Bimodal (Result)

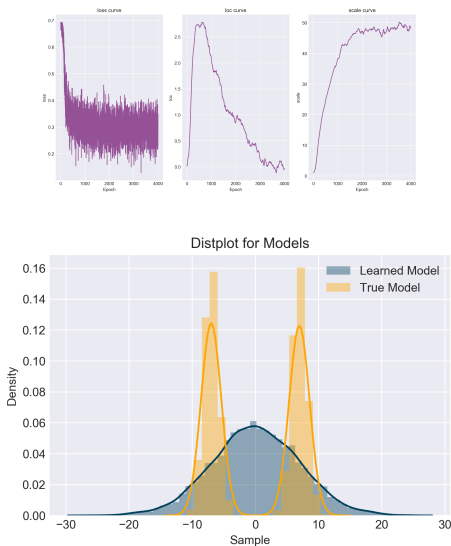


Figure: $Q \sim \mathcal{N}(-0.04, 48.20)$

Jensen - Shannon Divergence: Right Shift (Attempt 2)

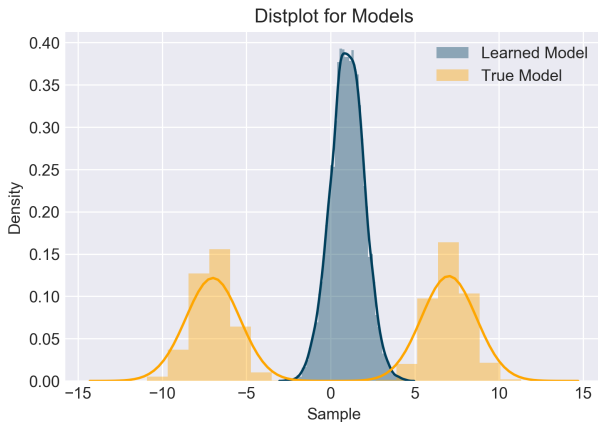


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(1, 1)$

Jensen - Shannon Divergence: Right Shift (Result)

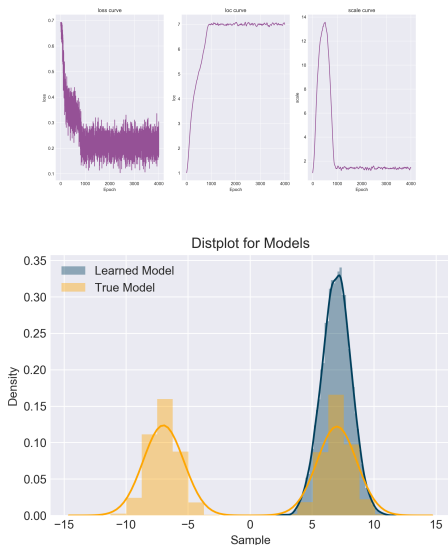


Figure: $Q \sim \mathcal{N}(6.99, 1.43)$

Jensen - Shannon Divergence: Left Shift (Attempt 3)

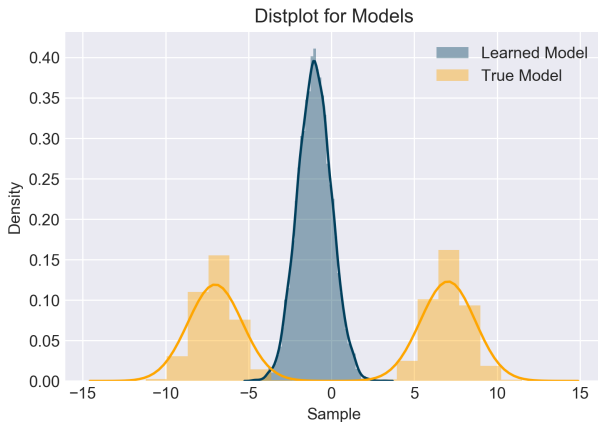


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(-1, 1)$

Jensen - Shannon Divergence: Left Shift (Result)

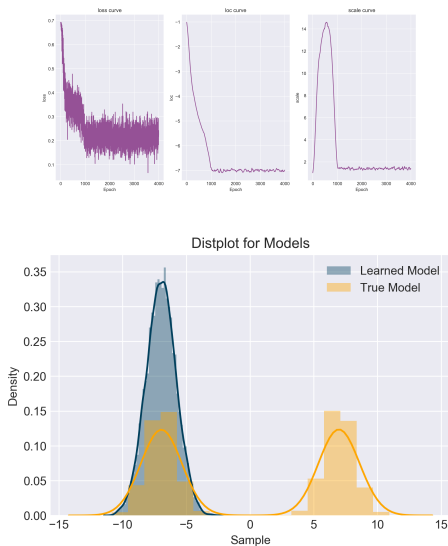


Figure: $Q \sim \mathcal{N}(-6.98, 1.38)$

Jensen - Shannon Divergence Loss

$$\text{JSD}(P \parallel Q) = \frac{1}{2}D_{KL}(P \parallel M) + \frac{1}{2}D_{KL}(Q \parallel M)$$
$$M = \frac{1}{2}(P + Q)$$

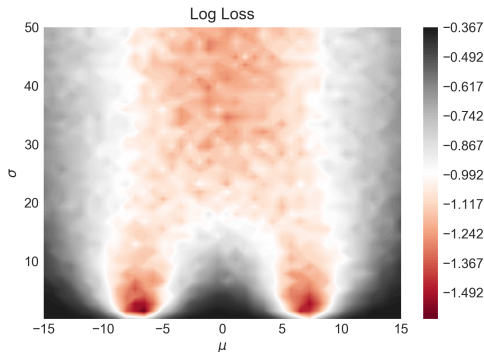


Figure: Loss Landscape for JS Divergence

A Family of Divergences: f -Divergence

- ▶ KL Divergence is a special case of the f -divergence
- ▶ The f -divergence is a family of divergences that can be written as:

$$D_f(P \parallel Q) = \int \overbrace{q(x)}^{\text{Weight}} f \left(\underbrace{\frac{p(x)}{q(x)}}_{\text{Odds Ratio}} \right) dx$$

A Family of Divergences: f -Divergence

$$D_f(P \parallel Q) = \int \underbrace{q(x)}^{\text{Weight}} \underbrace{f\left(\frac{p(x)}{q(x)}\right)}_{\text{Odds Ratio}} dx$$

Divergence	$f(t)$
Forward KL	$t \log t$
Reverse KL	$-\log t$
Hellinger Distance	$(\sqrt{t} - 1)^2, 2(1 - \sqrt{t})$
Total Variation	$\frac{1}{2} t - 1 $
Pearson χ^2	$(t - 1)^2, t^2 - 1, t^2 - t$
Neyman χ^2 (Reverse Pearson)	$\frac{1}{t} - 1, \frac{1}{t} - t$

Other Metrics: Earth Mover's Distance

Summary of Methods

	P		Q	
	$\log p(x)$	$x \sim P$	$\log q(x)$	$x \sim Q$
Cross-Entropy		✓	✓	
Forward KL	✓	✓	✓	
Reverse KL	✓		✓	✓
JS Divergence	✓	✓	✓	✓
f -Divergence	✓	✓	✓	✓

Potpourri: Advanced Techniques

	P		Q	
	$\log p(x)$	$x \sim P$	$\log q(x)$	$x \sim Q$
Cross-Entropy		✓	✓	
Forward KL	✓	✓	✓	
Reverse KL	✓		✓	✓
JS Divergence	✓	✓	✓	✓
f -Divergence	✓	✓	✓	✓
Adversarial		✓		✓

Potpourri: Advanced Techniques

1. Transforms
 - ▶ Normalizing Flow Models
2. Variational Inference
 - ▶ ELBO
3. Adversarial Training (Forest of GANs)
4. Markov Chain Monte Carlo
 - ▶ Metropolis-Hastings
 - ▶ Gibbs Sampling
 - ▶ Hamiltonian Monte Carol
 - ▶ NUTS